=> d his

(FILE 'HOME' ENTERED AT 07:57:32 ON 23 MAR 2004)
FILE 'CA' ENTERED AT 07:58:00 ON 23 MAR 2004
L1 2118 S (MASS(A)SPEC? OR MS(A)(TANDEM OR MS))AND((ION OR NEUTRAL)(1A)(LOSS OR LOST OR SERIES OR PAIR)OR(Y OR B)(W)ION)
L2 2 S L1 AND(MINE# OR MINING)
L3 74 S L1 AND((DATA OR SPECTRA# OR SPECTRUM)(4A)(REDUCT? OR DATABASE OR SEARCHING OR ALGORITHM OR INDEX? OR SCORE# OR SCORING OR MATCH? OR INTERPRET? OR RETRIEV?))
L4 9 S L1 AND((DATABASE OR DATA BASE)(4A)(REDUCT? OR DATABASE OR SEARCHING OR ALGORITHM OR INDEX? OR SCORE# OR SCORING OR MATCH? OR INTERPRET? OR RETRIEV?))
L5 58 S L2-4 NOT PY>2000
FILE 'BIOSIS' ENTERED AT 08:14:48 ON 23 MAR 2004
L6 12 S L5
FILE 'MEDLINE' ENTERED AT 08:15:39 ON 23 MAR 2004
L7 14 S L5
FILE 'CA, BIOSIS, MEDLINE' ENTERED AT 08:19:55 ON 23 MAR 2004
L8 61 DUP REM L5 L6 L7 (23 DUPLICATES REMOVED)

=> d bib,ab l8 1-61

L8 ANSWER 6 OF 61 CA COPYRIGHT 2004 ACS on STN
AN 132:319322 CA
TI De novo sequencing of proteins with **mass spectrometry** using the differential scanning technique
AU Wilm, M.; Neubauer, G.; Taylor, L.; Shevchenko, A.; Bachi, A.
CS European Molecular Biology Laboratory, Heidelberg, D-69012, Germany
SO Proteome and Protein Analysis (2000), 65-79. Editor(s): Kamp, Roza Maria; Kyriakidis, Dimitris; Choli-Papadopoulou, Theodora. Publisher: Springer-Verlag, Berlin, Germany.
AB A review with numerous refs. Protein identification in complete sequence **databases** or partial sequence **databases** is done preferentially by **mass spectrometric** techniques. However, protein de novo sequencing with **mass spectrometry** is more difficult to achieve. Generally, it is done by C-terminal labeling of the peptide. C-terminal fragment ions are identified in the tandem **mass spectrum** by the addnl. mass of the label. This very often allows to assign the correct amino acid sequence to a fragment spectrum of a tryptic peptide. When sub-isotopically resolved tandem **mass spectra** generated with a triple quadrupole machine are to be interpreted, methylation is the preferred labeling method since the mass shift is at least 14 Da. When working with a quadrupole time of flight machine which generates isotopically resolved fragment spectra, 50 % 18O labeling is the method of choice. In this article a method is presented, called differential scanning, which addresses the major limitations of methylation and 18O labeling preserving at the same time the sensitivity of the anal. For the triple quadrupole based de novo sequencing there is the need to do two sep. **tandem MS** investigations, one for the unmodified peptide mixt. and the second for the methylated one. For the quadrupole time of flight

based technique the difficulty is to clearly and unambiguously identify the 50 % 18O labeled fragment ions via their 1:1 16O/18O isotopic cluster in case of overlap with chem. noise ions and other ions mimicking the characteristic isotopic distribution. When the differential scanning technique is used addnl. information is generated to identify the C- terminal fragment ions. This information can be used to generate a simplified **y ions** only **tandem MS** spectrum and it can be exploited to improve computer algorithms to read out the amino acid sequence automatically.

L8 ANSWER 10 OF 61 CA COPYRIGHT 2004 ACS on STN
AN 130:121726 CA
TI Automated interpretation of high-energy collision-induced dissociation spectra of singly protonated peptides by 'seqMS', a software aid for De Novo sequencing by tandem **mass spectrometry**
AU Fernandez-de-Cossio, Jorge; Gonzalez, Javier; Betancourt, Lazaro; Besada, Vladimir; Padron, Gabriel; Shimonishi, Yasutsugu; Takao, Toshifumi
CS Center for Genetic Engineering and Biotechnology, Havana, Cuba
SO Rapid Communications in Mass Spectrometry (1998), 12(23), 1867-1878
AB SeqMS, a software program designed for the automated interpretation of high-energy collision-induced dissocn. (CID) **mass spectra** of singly protonated peptides ionized by fast atom bombardment, has been developed. The software is capable of probing the sequence of an unknown peptide, and even of certain modified peptides. The program, compiled for WINDOWS95 or NT, also permits the **retrieval** of raw **data** and the reconstruction of the spectra on a user-friendly graphical interface with the aid of several tools for processing the spectra, which include setting multiple threshold levels and automatic peak detection. SeqMS is capable of generating candidate sequences, based on the detected peaks, and of displaying the resulting assignments for each candidate in a spectrum or in tabular form. The software has the following capabilities: (1) the ions derived from backbone and side-chain fragmentations, internal and immonium ions, and side-chain **loss ions** can be used for calcn.; (2) 18O-labeling of a peptide at the C terminus, a methodol. which was developed to differentiate N-terminal from C-terminal ions, is applicable as an optional setting; (3) modified amino acids and N- or C-terminal blocking groups are taken into account for calcn. according to the user's setting in a library; (4) amino acid compn. and partial or complete amino acid sequence of a peptide can be used as input for calcn.; (5) the assignments of signal output in a spectrum can be graphically edited, and then re-calcd. based on the edited peaks. The efficacy of the program is demonstrated by testing 74 high-energy CID spectra, obtained using a four-sector instrument, of synthetic, proteolytic, and biol. active peptides, some of which contain modified groups.

L8 ANSWER 13 OF 61 CA COPYRIGHT 2004 ACS on STN
AN 129:105694 CA
TI The identification of peptide modifications derived from gel-separated proteins using electrospray triple quadrupole and ion trap analyses

AU Swiderek, Kristine M.; Davis, Michael T.; Lee, Terry D.
CS Beckman Research Inst., City Hope, Duarte, CA, USA
SO Electrophoresis (1998), 19(6), 989-997
AB Microspray tandem **mass spectrometry** (**MS/MS**) in combination with database search routines has become a powerful tool for the identification of proteins from femtomole amts. of material following gel electrophoresis and in-gel digestion procedures. Artifactual modification of susceptible residues can arise during gel electrophoresis, leading to unexpected peptide mass shifts during mass anal. Collision-induced dissocn. (CID) spectra generated from these derivatized peptides can defy direct **interpretation** by automated **database** search routines and remain unidentified. The authors evaluate the **MS/MS** spectra of peptides carrying oxidized derivs. of Trp and Met residues, and various modifications of Cys. The authors demonstrate that certain of these modifications generate characteristic fragmentation patterns or "fingerprints", during CID anal., the knowledge of which can facilitate the **interpretation** of the **spectra**. The authors show that these signature fragment ions are predominantly produced during the CID anal. of singly charged ions although they can be obsd. in the **MS/MS** spectra of the doubly charged species as well. In other cases, the CID spectrum lacks a characteristic fingerprint and the modification remains silent. CID spectra of related peptides, differing only by their modifications, are similar and all or part of the fragment ion spectra will have shifted by a discreet mass, which facilitates the identification of the modified residue. At the same time, the comparison of related spectra can prevent misinterpretations such as the assignment of a residue mass to the wrong amino acid or a **neutral loss** fragment **ion** to a y- or **b-ion**.

L8 ANSWER 26 OF 61 CA COPYRIGHT 2004 ACS on STN
AN 124:56531 CA
TI Charged vs. **neutral** nucleobase **loss** from multiply charged oligoribonucleotide anions
AU McLuckey, Scott A.; Vaidyanathan, Gopalakrishnan; Habibi-Goudarzi, Sohrab
CS Chemical and Analytical Sciences Division, Oak Ridge National Laboratory, Oak Ridge, TN, 37831-6365, USA
SO Journal of Mass Spectrometry (1995), 30(9), 1222-9
AB Tandem **mass spectra** of a variety of adenine-contg. deoxynucleic acid anions obtained using collisional activation in a quadrupole ion trap are described. Data are reported for singly charged mono-, di- and trinucleotide species, and also for multiply charged anions derived from tri-, tetra-, penta- and hexanucleotides. Attention is focused on the first step in the unimol. decompn. of these species, namely the loss of the nucleobase. Specifically, the competition between the loss of the nucleobase as a neutral vs. its loss as an anion is addressed within the context of a proposed proton-bound intermediate consisting of the nucleobase and a phosphodiester linkage. The **data** are **interpreted** on the basis of the energy surface involved in the break-up of the proton-bound intermediate, which can explain why the competition between loss of a neutral vs. charged base is strongly dependent upon

the charge of the parent ion.

L8 ANSWER 27 OF 61 CA COPYRIGHT 2004 ACS on STN
AN 124:217649 CA
TI An algorithm for molecular weight prediction from EI **mass spectra**
AU Yang, Boyu; Zhu, Damo; Hong, Qunfa; Sun, Guoqiang; Liu, Renyu; Liebich, Hartmut M.; Gesele, Elke
CS Dalian Institute of Chemical Physics, Dalian, 116011, Peop. Rep. China
SO Chinese Science Bulletin (1995), 40(13), 1087-9
AB The algorithm follows the flow chart: (1) low-resoln. EI **mass spectrum**; (2) isotope anal.; (3) detn. of MSP; (4) creation of **neutral loss** spectrum; (5) constraint of N2 gas; (6) calcn. of RF for each candidate; and (7) output by RF sequence.

L8 ANSWER 28 OF 61 CA COPYRIGHT 2004 ACS on STN
AN 123:187353 CA
TI Chemical substructure identification by **mass spectral** library **searching**
AU Stein, Stephen E.
CS NIST Mass Spectrometry Data Cent., Gaithersburg, MD, USA
SO Journal of the American Society for Mass Spectrometry (1995), 6(8), 644-55
AB A library-search procedure that identifies structural features of an unknown compd. from its electron-ionization **mass spectrum** is described. Like other methods, this procedure 1st **retrieves** library compds. whose **spectra** are most similar to the spectrum of an unknown compd. If then deduces structural features of the unknown compd. from the chem. structures of the retrievals. Unlike other methods, the significance of each **retrieved spectrum** is weighted according to its similarity to the spectrum of the unknown compd. Also, a peaks-in-common screening step serves to reduce search times and an optimized dot product function provides the match factor. If the mol. wt. of the unknown compd. is provided, the identification of certain substructures can be improved by including **neutral loss** peaks. Correlations between the presence of a substructure in a test searching the NIST/EPA/NIH ref. library with a 7891. compd. test set. These correlations allow the estn. of probabilities of substructure occurrence and absence in an unknown compd. from the results of a library search. This method may be viewed as an optimization of the K-nearest neighbor method of Isenhour and co-workers, with improvements that arise from spectrum screening, peak scaling, an optimal distance measure, a relative-distance weighting scheme, and a larger ref. library.

L8 ANSWER 31 OF 61 CA COPYRIGHT 2004 ACS on STN
AN 121:156944 CA
TI Establishment of an intelligent **mass spectral interpretation** system
AU Zhu, Damo; Yang, Boyu; Hong, Qunfa; Sun, Guoqiang; Xu, Chongde
CS Dalian Inst. Chem. Phys., Chin. Acad. Sci., Dalian, 116012, Peop. Rep. China
SO Fenxi Huaxue (1994), 22(3), 233-6
LA Chinese
AB A new development in five sections of the automatic structure

elucidation system/**mass spectrometry** (ASES/MS) system is discussed. In comparison with other systems, the ASES/MS system has three advantages: spectra in the data base have a high reliability; the system has a strong self-learning function; **neutral loss** rules are used systematically.

L8 ANSWER 36 OF 61 CA COPYRIGHT 2004 ACS on STN
AN 114:135337 CA
TI Exact mass probability based matching of high-resolution unknown **mass spectra**
AU Loh, Stanton Y.; McLafferty, Fred W.
CS Baker Chem. Lab., Cornell Univ., Ithaca, NY, 14853-1301, USA
SO Analytical Chemistry (1991), 63(6), 546-50
AB Unknown **mass spectra** measured with millimass accuracy can be matched (for quant. anal.) against a comprehensive unit-mass-resoln. data base of electron ionization spectra by utilizing its information on mol. elemental compns. and known correlations of common **neutral** species **lost** in **ion** dissocns. Adding this exact (E) mass capability to the probability-based matching (PBM) algorithm provides substantial performance improvements. Using matching criteria that retrieve 80% of the correct answers, EPBM increases the reliability of **retrieving** a **spectrum** of the same structure from 23% to 39%; accepting structural differences to which **mass spectrometry** is insensitive (class IV matches), EPBM increases the reliability from 44% to 71%, halving the no. of wrong answers. Similarly, for EPBM only 6% of best matches are incorrect (Class IV) vs. 10% by PBM.

L8 ANSWER 40 OF 61 CA COPYRIGHT 2004 ACS on STN
AN 104:141456 CA
TI New methods of **interpretation** of chromatographic-**mass spectrometric data**
AU Ioffe, B. V.; Zenkevich, I. G.
CS Chem. Dep., Leningrad State Univ., Leningrad, 199164, USSR
SO Journal of Chromatography (1985), 349(2), 385-93
AB It is proposed to carry out the group identification of org. substances according to low-resoln. **mass spectra** on the basis of the concept of a comparison of nos. of modulus 14. The concept of homologous groups is introduced. These groups are a total set of homologous series, the terms of which have mass nos. comparable in modulus 14. The nos. of homologous groups of mol. and fragment ions may serve as important diagnostic features for group identification according to the main peaks of the **mass spectrum**. The reliability and unequivocal character of group identification increase considerably if the total intensity of the peaks of each group is taken into account and averaged spectra of **ion series** are used for the characterization of classes of compds. When the spectra of **ion series** are compared, it is proposed to take into account std. deviations of peak intensities and to use as an addnl. classification feature homologous increments of retention indexes calcd. on the basis of the quatuordecimal system of calculus of mass nos.

L8 ANSWER 41 OF 61 CA COPYRIGHT 2004 ACS on STN
AN 98:64998 CA
TI Determination of drugs in blood serum by **mass spectrometry/mass spectrometry**
AU Brotherton, Harry O.; Yost, Richard A.
CS Dep. Chem., Univ. Florida, Gainesville, FL, 32611, USA
SO Analytical Chemistry (1983), 55(3), 549-53
AB A rapid, sensitive technique based on tandem **mass spectrometry** (**MS/MS**) for both screening and confirmation of drugs is described. This **MS/MS** technique replaces the chromatog. sepn. with a **mass spectrometric** sepn. and greatly reduces the amt. of sample prepn. required. It allows the simultaneous screening for as many as 50 drugs and metabolites in <5 min. The technique involves an initial screening by monitoring selected parent ion/daughter **ion pairs** for each targeted compd., or selected **neutral losses** characteristic of targeted classes of compds. Confirmation involves obtaining daughter spectra of the parent ions for all positives and **matching** them with library daughter **spectra** of the pure compds. Detection limits for most drugs, with 1 μL of blood serum placed on the solids probe, are in the low parts-per-million (ng/μL) range. A simple extn. of the serum reduces these detection limits to the low parts-per-billion (pg/μL) range.

L8 ANSWER 42 OF 61 CA COPYRIGHT 2004 ACS on STN
AN 98:98347 CA
TI An improved maximum likelihood method for classifying **mass spectral** data
AU Glinzer, O.; Severin, D.
CS Inst. Erdoelforsch., Hannover, D-3000, Fed. Rep. Ger.
SO International Journal of Mass Spectrometry and Ion Physics (1983), 47, 325-8
AB A max. likelihood multicategory classifier for classifying the **mass spectra** of hydrocarbons is presented, which is based on the peak intensities and utilizes a weighting of the features according to their selectivity. Investigations were performed on 2234 hydrocarbon **mass spectra**. High prediction and good stability against measurement errors were obtained with storage and time requirements suitable for minicomputers. Addnl. use of **neutral losses** proved to be advantageous, esp. in the case of classifying alkanes. Multicategory and binary classifiers are compared with respect to their information gain.

L8 ANSWER 43 OF 61 CA COPYRIGHT 2004 ACS on STN
AN 96:34325 CA
TI A computer search system for chemical structure elucidation based on low-resolution **mass spectra**
AU Lebedev, K. S.; Tormyshev, V. M.; Derendyaev, B. G.; Koptyug, V. A.
CS Sci. Inf. Cent. Mol. Spectrosc., Novosibirsk Inst. Org. Chem., Novosibirsk, 630090, USSR
SO Analytica Chimica Acta (1981), 133(4), 517-25
AB A computerized search which employs the data on the masses and relative abundances of spectral peaks and primary **neutral losses** is designed for computer elucidation of chem. structures. Recognition of structural

fragments is based on anal. of the structures of ref. compds. selected as best **matches** to the **mass spectrum** of the compd. under investigation. Tests of the system on 67 unknown compds. show that the probability of recognizing a large structural fragment is 60-80%, depending on the fragment size (100-50% of mol. wt.), and that the reliability of the corresponding structural conclusion is 98%. An approach to automatic selection of the substructure common to all or several of the selected compds. is discussed.

L8 ANSWER 45 OF 61 CA COPYRIGHT 2004 ACS on STN
AN 94:56811 CA
TI Computer prediction of molecular weights from **mass spectra**
AU Mun, In Ki; Venkataraghavan, Rengachari; McLafferty, Fred W.
CS Dep. Chem., Cornell Univ., Ithaca, NY, 14853, USA
SO Analytical Chemistry (1981), 53(2), 179-82
AB The best-**matching spectra** found by the self-training interpretive and retrieval system (STIRS) exhibit primary **neutral loss** data resembling those of an unknown spectrum; this information is utilized in a computer program which predicts the mol. wt. of the unknown. Sep. predictions are made assuming that the mol. ion is, or is not, present. The spectral data used by STIRS for the former case include corresponding primary **neutral losses**, while for the latter case they include secondary **neutral losses matched** against ref. **spectra** that do not contain mol. ions. Such data are also used to choose which set of predictions is more reliable. For randomly selected unknowns, (15% with no mol. ion), the first choice of mol. wts. is correct in 91% and the first or second in 95% of the cases.

L8 ANSWER 48 OF 61 CA COPYRIGHT 2004 ACS on STN
AN 90:202955 CA
TI **Mass spectral** library searches using **ion series** data compression
AU Rasmussen, Gregory T.; Isenhour, T. L.; Marshall, John C.
CS Dep. Chem., Univ. North Carolina, Chapel Hill, NC, USA
SO Journal of Chemical Information and Computer Sciences (1979), 19(2), 98-104
AB A series of library searches using a **mass spectral** data compression method based on fractional ion currents of specific **ion series** is described. The method offers efficient data compression, reasonable search performance, and a capability for use with file partitioning to reduce search times.

L8 ANSWER 49 OF 61 CA COPYRIGHT 2004 ACS on STN
AN 90:114533 CA
TI SISCOM - a new library search system for **mass spectra**
AU Damen, H.; Henneberg, D.; Weimann, B.
CS Max-Planck-Inst. Kohlenforsch., Muelheim/Ruhr, Fed. Rep. Ger.
SO Analytica Chimica Acta (1978), 103(4), 289-302
AB SISCOM is a library search system for **mass spectrometry** which is based on a new method of coding spectra by selecting the most important peaks within homologous **ion series**, and on a multiple factor assessment of the result. Examples demonstrate the ability of the system to identify

various compds., even from mixts. or by ref. spectra which differ from those measured. SISCOM is esp. suitable for detecting structural similarities like common substructures, even in cases where no similarity can be recognized by visual comparison of patterns or by human **interpretation** of the **spectrum**.

L8 ANSWER 51 OF 61 CA COPYRIGHT 2004 ACS on STN
AN 85:93151 CA
TI Simple **index** for classifying **mass spectra** with applications to fast library searching
AU Dromey, R. Geoff
CS Res. Sch. Chem., Aust. Natl. Univ., Canberra, Australia
SO Analytical Chemistry (1976), 48(11), 1464-9
AB A simple **ion series**-related index was developed for classifying **mass spectra**. The index restricts the choice of mol. classes to which a spectrum may belong. Intraclass variations can be correlated with structural differences, while interclass variations are derived from the influence of different functional groups. The specificity of the index makes it ideal for structuring and **searching mass spectral** libraries. A library search scheme which retains the class definition of the file and still yields close to an order of magnitude redn. in the search space is described.

L8 ANSWER 52 OF 61 CA COPYRIGHT 2004 ACS on STN
AN 86:54496 CA
TI Computer-aided **interpretation** of **mass spectra**. Part XIII. Increased information from **neutral loss** data
AU Dayringer, Henry E.; McLafferty, F. W.; Venkataraghavan, Rengachari
CS Dep. Chem., Cornell Univ., Ithaca, NY, USA
SO Organic Mass Spectrometry (1976), 11(8), 895-900
AB Improvements in the 'Self-training interpretive and retrieval system' for identification of unknown **mass spectra** are reported by modifications of the data classes using information on the masses of **neutral** fragments **lost** from the mol. ion. Modifications include use of overlapping mass ranges, sets of homologous series of losses, and an arithmetic combination of the data class rankings to give an 'overall **match** factor' for **neutral loss data**.

L8 ANSWER 55 OF 61 CA COPYRIGHT 2004 ACS on STN
AN 82:105973 CA
TI Computer based search and **retrieval** system for rapid **mass spectral** screening of samples
AU Gronneberg, T. O.; Gray, N. A. B.; Eglinton, G.
CS Sch. Chem., Bristol Univ., Bristol, UK
SO Analytical Chemistry (1975), 47(3), 415-19
AB An on-line lab. computer system that attempts to det. the chem. class of each component in a gas chromatog.-**mass spectroscopy** run as data are acquired is described. This preliminary orientation is followed by a non-real time file search against automatically-chosen specialized ref. files. Either **ion-series** classification or a "profile" is used for the mapping of an unknown onto the appropriate ref. file for spectrum

identification. The files each contain only the spectra of compds. of similar structures. The search files do not contain the common ions but rather those ions which distinguish each ref. compd. from other similar structures. Few comparisons have to be made, and the identifications are normally more precise because distinctive ions are used. Ref. files are built up by selecting stds. from constituents of the complex mixts. under study; this procedure ensures that the files are appropriate for the anal. problem.

L8 ANSWER 56 OF 61 CA COPYRIGHT 2004 ACS on STN
AN 79:59045 CA
TI Computer-aided **interpretation** of **mass spectra**. III. Self-training **interpretive** and retrieval system
AU Kwok, Kain-Sze; Venkataraghavan, Rengachari; McLafferty, F. W.
CS Dep. Chem., Cornell Univ., Ithaca, NY, USA
SO Journal of the American Chemical Society (1973), 95(13), 4185-94
AB A self-training system is described for computer **interpretation** of **mass spectra** which utilizes directly data of all available ref. spectra, and does not require prior spectra-structure correlations of these data either by human or computer effort. The computer selects different classes of data known to have high structural significance, such as characteristic **ions**, **series** of **ions**, and masses of **neutrals lost**, from the unknown **mass spectrum**, and **matches** these against the corresponding **data** of all the ref. spectra. The ref. compds. of closest **match** in each **data** class are examd. for common structural features; criteria were detd. so that such features can be identified with ~95% reliability. Tests with 110 "unknowns" not represented in the ref. file showed that extensive-to-complete structural information can be obtained, if spectra of related compds. are present in the ref. file.

L8 ANSWER 57 OF 61 CA COPYRIGHT 2004 ACS on STN
AN 76:80833 CA
TI Compound classifier based on computer analysis of low-resolution **mass spectral** data. Geochemical and environmental applications
AU Smith, Dennis H.
CS Sch. Chem., Bristol Univ., Bristol, UK
SO Analytical Chemistry (1972), 44(3), 536-47
AB A computer-based method for detn. of chem. compd. class based on low resolution **mass spectral** data was developed. The method relies on computer anal. of sets of std. spectra, reducing these large data sets to a much smaller correlation set. The correlation set, consisting of **ion series** spectra of each class, is used in subsequent automatic computer classification of **mass spectra**. This approach is particularly important in anal. of data from coupled gas chromatograph/**mass spectrometer** systems where large nos. of spectra of sepd. components of complex mixts. can be classified rapidly and further structural information elicited based on this classification. Although initially programmed for compd. classes relevant to geochem. and environmental studies, the correlation set and structural information programs can easily be expanded to include classes important in other areas of research. The simplicity of the method lends itself readily to small

computer or semiautomatic methods of **data redn.** and anal.

L8 ANSWER 59 OF 61 CA COPYRIGHT 2004 ACS on STN
AN 70:77120 CA
TI Computer-aided **interpretation** of **mass spectra**
AU Venkataraghavan, Rengachari; McLafferty, Fred W.; Van Lear, George E.
CS Purdue Univ., Lafayette, IN, USA
SO Organic Mass Spectrometry (1969), 2(1), 1-15
AB A system is described in which computer techniques are used to carry out major steps in the procedure for **interpretation** of high-resolution **mass spectral** data. These steps include identification and evaluation of the mol. ion, **neutral** fragments **lost** from the mol. ion, and characteristic **ion series**, followed by elucidation of specific structural details using a sub-routine for the particular compd. class selected. The technique shows promise of not only increasing the interpreter's efficiency, but of providing more specific and detailed structural information from the spectral data.

L8 ANSWER 61 OF 61 CA COPYRIGHT 2004 ACS on STN
AN 63:7394 CA
OREF 63:1312a-d
TI Application of **mass spectrometry** to structure problems. XXVI. Computer-aided **interpretation** of high-resolution **mass spectra**
AU Biemann, K.; McMurray, W. J.
CS Massachusetts Inst. of Technol., Cambridge
SO Tetrahedron Letters (1965), (11), 647-53
AB cf. CA 61, 10161g; 62, 10474b, 14737f. A no. of criteria which uniquely det. the mol. ion can be set if the spectrum is obtained with a spectrometer of resolving power permitting detn. of the elemental compn. of all the ions. The species may not contain any heavy isotopes; the no. of H atoms must be even if the no. of N atoms is even or zero, and must be odd if the no. of N atoms is odd; and the mass difference between the mol. ion and the ions of lower mass must correspond to a combination of atoms that can be lost in a reasonable fragmentation process. If the peak of highest mass and not contg. heavy isotopes does not fulfill these criteria, the mol. compn. of the compd. must differ from these ions by a combination of atoms that can be lost in a simple fragmentation process, and the elemental compn. of the ions of mass lower than the mol. ion must not exceed for any one element the compn. of the mol. ion. These decisions are readily made by computer, and the FORTRAN program based on these criteria was written. As an example, the conclusions arrived at by the computer when processing the high-resolution spectrum of androsterone acetate were tabulated and correctly represented the best fit out of 5 ions at the high-mass end, all of which could be mol. ions based on their elemental compn. alone. Addnl. structural information obtained simultaneously was tabulated. The predominance of **ions** involving **loss** of AcOH and Me strongly suggested the presence of an AcO group as well as Me attached to a highly substituted C atom. The loss of CO in various steps agreed with a cyclic ketonic structure.

=> log y
STN INTERNATIONAL LOGOFF AT 08:20:44 ON 23 MAR 2004